

Testing the nonlocal kinetic energy functional of an inhomogeneous, two-dimensional degenerate Fermi gas within the average density approximation

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(Dated: July 14, 2015)

In a recent paper [Phys. Rev. A **89**, 022503 (2014)], the average density approximation (ADA) was implemented to develop a parameter-free, nonlocal kinetic energy functional to be used in the orbital-free density-functional theory of an inhomogeneous, two-dimensional (2D), Fermi gas. In this work, we provide a detailed comparison of self-consistent calculations within the ADA with the exact results of the Kohn-Sham density-functional theory, and the elementary Thomas-Fermi (TF) approximation. We demonstrate that the ADA for the 2D kinetic energy functional works very well under a wide variety of confinement potentials, even for relatively small particle numbers. Remarkably, the TF approximation for the kinetic energy functional, *without any gradient corrections*, also yields good agreement with the exact kinetic energy for all confining potentials considered, although at the expense of the spatial and kinetic energy densities exhibiting poor point-wise agreement, particularly near the TF radius. Our findings illustrate that the ADA kinetic energy functional yields accurate results for *both* the local and global equilibrium properties of an inhomogeneous 2D Fermi gas, without the need for any fitting parameters.

PACS numbers: 31.15.E-, 71.15.Mb, 03.75.Ss, 05.30.Fk

I. INTRODUCTION

In a recent paper [1], the average density approximation (ADA) was used to construct a manifestly nonlocal kinetic energy (KE) functional for a two-dimensional (2D), inhomogeneous Fermi gas at zero-temperature. The motivation behind this work was to provide an improved, orbital-free density-functional theory (DFT) [2] beyond the 2D Thomas-Fermi von Weizsäcker (TFvW) theory, which relies upon an adjustable parameter, the von Weizsäcker (vW) coefficient, λ_{vW} , for its implementation [3, 4]. Owing to the fact that the TFvW parameter needs to be fine-tuned depending on the problem under consideration, the TFvW theory has the undesirable feature of not being universally applicable to an arbitrary inhomogeneous system. More importantly, in 2D, the TFvW theory is completely *ad hoc*, with no formal justification within the usual gradient expansion techniques [4–11].

While the ADA KE functional was shown in [1] to yield superlative agreement with the exact results available for harmonic confinement, it is not immediately clear if similar agreement will be found for other potentials [14, 15]. In this paper, we will examine the efficacy of the 2D KE functional under a variety of confinement potentials, *via* fully self-consistent calculations for the noninteracting system. Our focus on the noninteracting system allows us to compare our ADA calculations with the results obtained within the Kohn-Sham (KS) DFT [2], where the noninteracting KE is treated *exactly*.

To this end, the rest of our paper is organized as follows. In the next section, we briefly review the ADA approach for constructing the 2D KE functional, and generalize our earlier results [1] to also include the case of fully spin-polarized Fermi gas. In Sec. III, we present self-consistent calculations under various confinement potentials, and compare the spatially dependent and integrated equilibrium properties with the exact KS DFT and the Thomas-Fermi (TF) approximation. Our central finding is that the ADA KE functional yields good agreement for both the local and global equilibrium properties of a 2D inhomogeneous Fermi gas, with no adjustable parameters. Finally, in Sec. IV, we present our closing remarks and directions for future work.

II. THE ADA AND TFW-LIKE THEORY

The details of the derivation of the 2D nonlocal KE functional within the ADA have already been presented in Ref. [1]. Here, we will provide a simple generalization of this result, so that it may also be applicable to a spin-polarized Fermi gas. In order to take the spin degeneracy, g , into account ($g = 1$ or $g = 2$), we need only introduce the following generalized quantities, all in 2D (hereby, we take $\hbar = m = 1$ unless otherwise noted), *viz.*, the Fermi

wave vector,

$$|\mathbf{k}_F| = k_F = \sqrt{\frac{4\pi\rho}{g}} , \quad (1)$$

the KE per particle for the uniform system,

$$t_0 = \frac{\pi}{g}\rho , \quad (2)$$

and the static response function,

$$\chi_0(\eta) = -\frac{g}{2\pi} \begin{cases} 1, & \eta < 1 , \\ 1 - \sqrt{1 - \frac{1}{\eta^2}}, & \eta \geq 1 , \end{cases} \quad (3)$$

with

$$\eta \equiv \frac{|\mathbf{k}|}{2k_F} , \quad (4)$$

and \mathbf{k} is the wave vector conjugate to $\mathbf{r} - \mathbf{r}'$. Following the analysis carried out in Ref. [1] leads to the 2D nonlocal KE functional within the ADA, *viz.*,

$$T_{\text{ADA}}[\rho] = \frac{3\pi}{2g} \int d^2r \int d^2r' \rho(\mathbf{r}') \tilde{w}(\mathbf{r} - \mathbf{r}'; \rho(\mathbf{r})) \rho(\mathbf{r}) - \frac{1}{2} T_{\text{TF}}[\rho] + T_{\text{vW}}[\rho] , \quad (5)$$

where the vW KE functional is given by [16]

$$T_{\text{vW}}[\rho] = \frac{1}{8} \int d^2r \frac{|\nabla \rho(\mathbf{r})|^2}{\rho(\mathbf{r})} , \quad (6)$$

and $T_{\text{TF}}[\rho]$ is the TF KE functional, which reads

$$T_{\text{TF}}[\rho] = \frac{\pi}{g} \int d^2r \rho(\mathbf{r})^2 . \quad (7)$$

The quantity, $\tilde{w}(\mathbf{r} - \mathbf{r}'; \rho(\mathbf{r}))$ in Eq. (5) is the real-space nonlocal weight function [1], whose Fourier transform takes the form $\tilde{w}(\eta) \equiv \frac{2}{3}w_0 + \frac{1}{3}$, where

$$\begin{aligned} w_0(\eta) &= [4\eta^2 \ln \eta + 1 + (\ln 4 - 3)\eta^2] \Theta(1 - \eta) \\ &+ \left[2\eta\sqrt{\eta^2 - 1} + \eta^2(\ln 4 - 2) - 2\eta^2 \ln \left(1 + \sqrt{1 - \frac{1}{\eta^2}} \right) \right] \Theta(\eta - 1) , \end{aligned} \quad (8)$$

and $\Theta(\cdot)$ is the Heaviside distribution.

The total energy functional is then given by

$$\begin{aligned} E_{\text{ADA}}[\rho] &= \frac{3}{g} \int d^2r \int d^2r' \frac{\pi}{2} \rho(\mathbf{r}') \tilde{w}(\mathbf{r} - \mathbf{r}'; \rho(\mathbf{r})) \rho(\mathbf{r}) - \frac{1}{g} \int d^2r \frac{\pi}{2} \rho(\mathbf{r})^2 + \frac{1}{8} \int d^2r \frac{|\nabla \rho(\mathbf{r})|^2}{\rho(\mathbf{r})} \\ &+ E_{\text{int}}[\rho(\mathbf{r})] + \int d^2r v_{\text{ext}}(\mathbf{r}) \rho(\mathbf{r}) , \end{aligned} \quad (9)$$

where $v_{\text{ext}}(\mathbf{r})$ is some external potential, and $E_{\text{int}}[\rho(\mathbf{r})]$ encodes all of the interactions. Note that for $g = 2$ (unpolarized), we obtain the results presented in Ref. [1]. Taking $g = 1$ would be appropriate for investigating the fully spin-polarized Fermi gas.

The variational minimization of Eq. (9) for a fixed number of particles yields the defining equations for what we

have called the Thomas-Fermi von Weizsäcker-like (TFvW-like) theory, *viz.*,

$$-\frac{1}{2}\nabla^2\psi(\mathbf{r}) + v_{\text{eff}}(\mathbf{r})\psi(\mathbf{r}) = \mu\psi(\mathbf{r}) , \quad (10)$$

where we have introduced the vW wave function, $\psi(\mathbf{r}) \equiv \sqrt{\rho(\mathbf{r})}$, and

$$v_{\text{eff}}(\mathbf{r}) = -\frac{\pi}{g}\psi(\mathbf{r})^2 + \phi(\mathbf{r}) + v_{\text{ext}}(\mathbf{r}) + \frac{\delta E_{\text{int}}}{\delta\rho(\mathbf{r})} , \quad (11)$$

$$\phi(\mathbf{r}) = \frac{3\pi}{2g} \int \frac{d^2k}{(2\pi)^2} \int d^2r_1 e^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}_1)} \left[\Omega\left(\frac{k}{2k_F(\mathbf{r})}\right) + \tilde{w}\left(\frac{k}{2k_F(\mathbf{r}_1)}\right) \right] \rho(\mathbf{r}_1) , \quad (12)$$

$$F(\eta) = \begin{cases} 1, & \eta < 1 , \\ \frac{1}{1 - \sqrt{1 - \frac{1}{\eta^2}}}, & \eta \geq 1 , \end{cases} \quad (13)$$

$$\Omega(\eta) \equiv \frac{2}{3} \left(F(\eta) + \frac{1}{2} - 2\eta^2 \right) . \quad (14)$$

Note that we have made the local approximation, namely, $k_F \rightarrow k_F(\mathbf{r}) = \sqrt{4\pi\rho(\mathbf{r})/g}$ and $\eta \rightarrow \eta(\mathbf{r}) = k/2k_F(\mathbf{r})$. The normalization to the desired particle number, N , determines the chemical potential, μ ,

$$N(\mu) = \int d^2r |\psi(\mathbf{r})|^2 . \quad (15)$$

The numerical solution of the TFvW-like self-consistent equations is discussed in Ref. [1]. In what follows, we shall denote the self-consistent (SC) ADA equilibrium spatial density by $\rho_{\text{sc}}(\mathbf{r})$.

III. COMPARISON WITH EXACT KOHN-SHAM CALCULATIONS

By its definition, the KS kinetic energy functional $T_{\text{KS}}[\rho]$ of N -independent particles is (recall that $g = 1, 2$)

$$T_{\text{KS}}[\rho] = g \sum_{i=1}^{N/g} \int d^2r \phi_i^*(\mathbf{r}) \left(-\frac{1}{2}\nabla^2 \right) \phi_i(\mathbf{r}) . \quad (16)$$

The $\phi_i(\mathbf{r})$ are single-particle orbitals, each satisfying a Schrödinger-like equation *viz.*,

$$-\frac{1}{2}\nabla^2\phi_i(\mathbf{r}) + v_{\text{eff}}(\mathbf{r})\phi_i(\mathbf{r}) = \varepsilon_i\phi_i(\mathbf{r}) , \quad i = 1, \dots, N \quad (17)$$

where the effective potential is given by

$$v_{\text{eff}}(\mathbf{r}) \equiv \frac{\delta E_{\text{int}}[\rho]}{\delta\rho(\mathbf{r})} + v_{\text{ext}}(\mathbf{r}) . \quad (18)$$

The ground state density is obtained from

$$\rho(\mathbf{r}) = g \sum_{i=1}^{N/g} \phi_i^*(\mathbf{r})\phi_i(\mathbf{r}) , \quad (19)$$

which at self-consistency, integrates to the total number of particles, N . For a noninteracting system, the KS theory is *exact*. Note that for $g = 2$, we require an even number of fermions. Furthermore, we also assume that the orbitals,

$\phi_i(\mathbf{r})$, are fully occupied. As seen in Tables I-V below, the requirement that the orbitals be fully occupied results in our KS calculations only being applicable to specific particle numbers, depending on the confinement potential.

In what follows, we will take $g = 2$, and compare the ADA equilibrium solutions for the noninteracting system with the self-consistent KS calculations, and the TF approximation. We will examine the total energy, the KE, as well as the quality of the equilibrium spatial and KE densities (*i.e.*, a point-wise comparison), in order to determine how well the ADA performs under a wide variety of confinement potentials. The inclusion of interactions will not alter the general results found in this paper, since in either the TFvW-like, KS, or TF DFT, the same level of approximation is made for the interaction energy functional, $E_{\text{int}}[\rho]$ (*e.g.*, the Hartree-Fock approximation [2, 12, 13]).

A. Power-law potentials

We take as our form for the power-law potential:

$$v_{\text{ext}}(r) = \frac{1}{2} V_0 r^\alpha, \quad (20)$$

where α is a positive integer. Here, we retain our fundamental constants (\hbar and m), and rather opt to scale all lengths and energies by $\ell = (\hbar^2/mV_0)^{1/(2+\alpha)}$ and $\hbar^2/m\ell^2$, respectively. For example, with $\alpha = 2$, and identifying $V_0 = m\omega_0^2$, we obtain the usual harmonic oscillator (HO) length and energy scales. For power-law potentials, Eq. (20), the virial theorem yields,

$$T = \frac{\alpha}{2} V, \quad (21)$$

which results in the total energy, E , being given by $E = (1 + 2/\alpha)T$. We may therefore focus our attention to a calculation of just the KE for power-law potentials.

In Tables I-IV, we compare the exact KS energies with the ADA results, for $\alpha = 2, 4, 6, 8$, respectively, and several particle numbers. We have also included an evaluation of $T_{\text{TF}}[\rho_{\text{TF}}]$, where $T_{\text{TF}}[\rho]$ is given by Eq. (7) and the TF energy functional is given by,

$$E_{\text{TF}}[\rho] = T_{\text{TF}}[\rho] + \int d^2r v_{\text{ext}}(\mathbf{r})\rho(\mathbf{r}). \quad (22)$$

A variational minimization of Eq. (22) with respect to a fixed number of particles yields the TF density, $\rho_{\text{TF}}(r)$, which in scaled units (hereby denoted by tildes) reads

$$\tilde{\rho}_{\text{TF}}(\tilde{r}) = \frac{1}{\pi} \left(\tilde{\mu}_{\text{TF}} - \frac{1}{2} \tilde{r}^\alpha \right) \Theta(\tilde{R} - \tilde{r}), \quad (23)$$

where \tilde{R} is the TF radius and $\Theta(x)$ is the Heaviside distribution. Note that Eq. (21) is also obeyed in the TF approximation.

Table I illustrates the agreement between the ADA, TF, and KS calculations under harmonic confinement ($\alpha = 2$). It is clear that the nonlocal ADA KE functional performs quite well at reproducing the total energy of the system, even for as few as $N = 2$ particles. Here, we have used the relative percentage error (RPE),

$$\text{RPE} \equiv \frac{|E_{\text{KS}} - E|}{E_{\text{KS}}}, \quad (24)$$

to quantify the agreement. In Eq. (24), E denotes the total energy calculated within the appropriate approximation (*i.e.*, the ADA or TF approximation). It is evident from Table I that both the ADA and TF KE energies approach the KS KE energy as $N \rightarrow \infty$ [1]. Note that for the isotropic HO in 2D, the particle numbers in Table I correspond to the case of *closed shells*. It is also worthwhile pointing out just how well the TF approximation (*i.e.*, local-density approximation) does at giving the kinetic energy. In fact, excluding $N = 6$, the TF approximation yields better results for the KE (compare the last two columns in Table I) than the ADA, in spite of the fact that the TF spatial density, Eq. (23), possesses an unphysical sharp drop to zero at the TF radius, $\tilde{R} = \sqrt{2}N^{1/4}$ with $\alpha = 2$.

We can try to gain some insight into the nature of the two approximations by examining the spatial dependence of the particle density for small particle numbers under harmonic confinement, illustrated in Fig. 1. The most notable feature is how inadequate the TF density (dashed curve) is compared to the exact KS density (solid curve), especially in the low density region. Indeed, the TF density is a monotonically decreasing function of position regardless of the

N	T_{KS}	$T_{\text{ADA}}[\rho_{\text{sc}}]$	$T_{\text{TF}}[\rho_{\text{TF}}]$	RPE^{ADA}	RPE^{TF}
2	1	1.07	0.94	7.0	6.0
6	5	4.93	4.90	1.4	2.0
12	14	13.74	13.86	1.9	1.0
20	30	29.51	29.81	1.6	0.63
30	55	54.28	54.77	1.3	0.4
90	285	283.16	284.61	0.64	0.14
132	506	503.60	505.52	0.47	0.09
182	819	816.11	818.44	0.35	0.07
420	2870	2866.48	2869.15	0.12	0.03

TABLE I: Comparison of the $\alpha = 2$ exact KS kinetic energy, T_{KS} , with the kinetic energy obtained from $T_{\text{ADA}}[\rho_{\text{sc}}]$, and $T_{\text{TF}}[\rho_{\text{TF}}]$. The last two columns give the relative percentage error (RPE) between T_{KS} and $T_{\text{ADA}}[\rho_{\text{sc}}]$ and T_{KS} and $T_{\text{TF}}[\rho_{\text{TF}}]$, respectively. Energies are measured in units of $\hbar^2/m\ell^2 = \hbar\omega_0$ for the 2D isotropic harmonic oscillator.

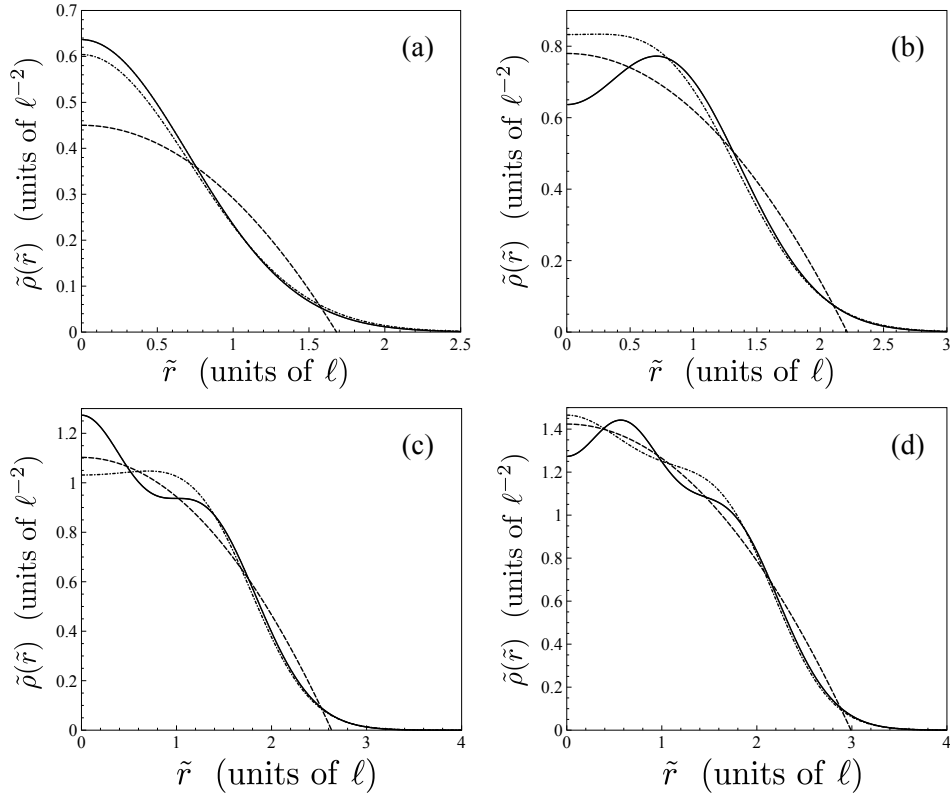


FIG. 1: The spatial density, $\tilde{\rho}(\tilde{r})$ (scaled units) for the KS (solid curve), ADA (dot-dashed curve) and TF (dashed curve) evaluated at (a) $N = 2$, (b) $N = 6$, (c) $N = 12$ and (d) $N = 20$ particles with $\alpha = 2$. All quantities have been scaled as discussed in the text.

particle number, a property clearly not shared by the ADA densities for $N > 6$. Moreover, the ADA (dot-dashed curve) provides excellent agreement with the KS density in the tail region. In the bulk, both the ADA and TF approximation fail to reproduce the oscillations in the KS KE density, although by $N = 20$, the ADA density shows signs of oscillatory structure, which while not directly attributable to the shell fillings, is at least encouraging. It is also interesting to note that both the ADA and TF densities at the centre of the trap alternately lie below or above the KS density as one moves from panels (a)-(d). The main message to be taken from Fig. 1 is that good agreement for the energy (a global property) does not imply that the spatial density will be likewise accurate; to wit, the TF approximation is far superior for obtaining the KE for $N > 20$, but fails completely to capture the surface profile of

the quantum mechanical density, which is characterized by the low density regime.

In Fig. 2, we present the KE densities under harmonic confinement for the same number of particles in Fig. 1. We have plotted $\tilde{r}\tilde{\tau}$ as this reflects the weighting of the radial variable in the integral for calculating the KE. It is immediately clear that the ADA provides a much better description of the KE density than the TF approximation. Indeed, for $N = 2$ in panel (a), the TF KE density is remarkably poor, while the ADA more closely follows the exact KS KE density, especially in the low-density region, where the ADA is noticeably superior to the TF approximation. As one moves up in particle number, the TF profile remains qualitatively the same, while the ADA starts to show signs of the oscillatory structure present in the KS KE density. Figure 2 once again illustrates that simply examining the KE itself *is not* sufficient to determine the efficacy of any proposed KE functional. For example, in panel (a), in spite of the TF KE density being noticeably inferior, the KE it yields is actually *better* than the ADA KE.

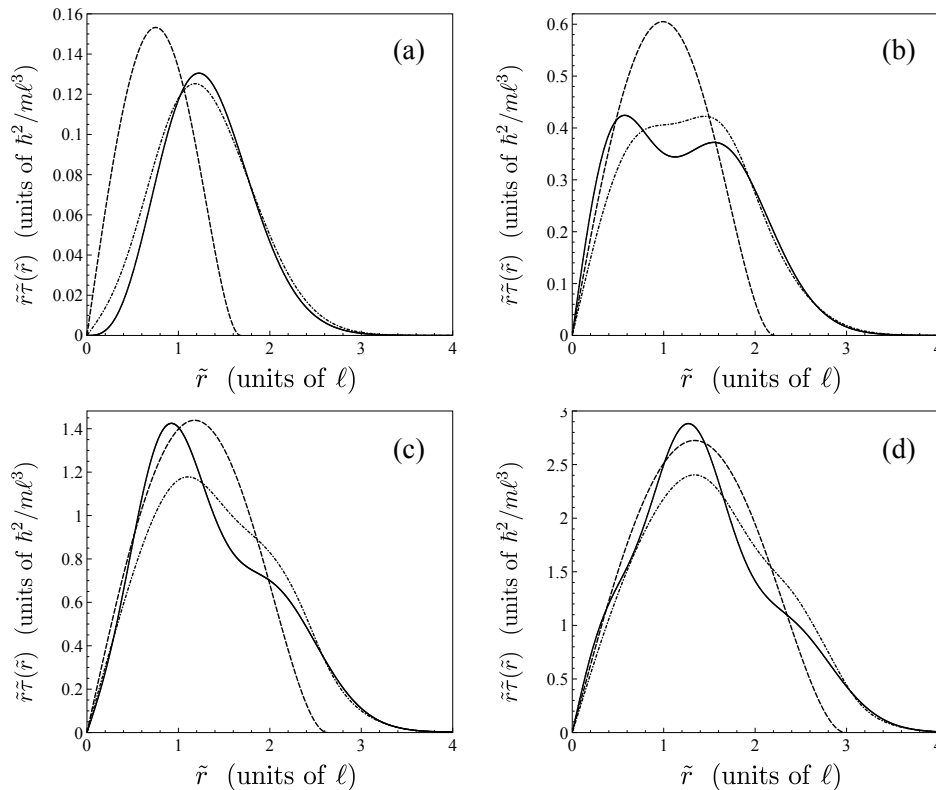


FIG. 2: The kinetic energy density, $\tilde{r}\tilde{\tau}(\tilde{r})$ (scaled units) for the KS (solid curve), ADA (dot-dashed curve) and TF (dashed curve) evaluated at (a) $N = 2$, (b) $N = 6$, (c) $N = 12$ and (d) $N = 20$ particles with $\alpha = 2$.

In Tables II-IV, we present the analogous data to Table I, but now for $\alpha = 4, 6, 8$, respectively. Let us first examine Table II, for which $\alpha = 4$. In contrast to $\alpha = 2$ in Table I, the ADA is now much closer to the exact KS KE energy, for a similar number of particles. However, as the particle number grows, the TF approximation once again provides a better value for the exact KS KE, and by $N = 300$, the TF approximation actually outperforms the ADA quite significantly.

An examination of the spatial density distribution (Fig. 3) reveals that even though the TF approximation yields reasonable agreement with the exact KS KE, it is an exceedingly poor representation of the exact spatial density (solid curves). Indeed, for $N = 2$, the TF approximation (dashed curve) shares almost no features of the exact density, while the ADA (dot-dashed curve) does an admirable job, especially in the tail region. In addition, the TF densities in Fig. 3 appear to be much worse than for the HO confinement, which is perhaps expected given that the TF approximation for the density is only valid for weakly inhomogeneous potentials. In other words, as α is increased, the potential provides a very tight confinement, and as a result, the spatial TF density is unsurprisingly inferior.

Similarly, in Fig. 4 we present the KE densities and observe the unsatisfactory behaviour of the TF approximation (dashed curves). In contrast, the ADA KE density (dot-dashed curves) is in very good agreement with the exact KS KE density (solid curves), including the oscillatory structure, particularly in panel (c), where the agreement is outstanding.

Tables III and IV correspond to $\alpha = 6, 8$, respectively, and follow the general trends observed in Table II. For this

N	T_{KS}	$T_{\text{ADA}}[\rho_{\text{sc}}]$	$T_{\text{TF}}[\rho_{\text{TF}}]$	RPE^{ADA}	RPE^{TF}
2	1.56	1.70	1.32	9.0	15
6	8.76	8.69	8.24	0.80	5.9
10	20.66	19.63	19.31	5.0	6.5
12	27.01	26.38	26.17	2.3	3.1
16	44.14	42.268	42.265	4.3	4.3
20	62.55	61.06	61.30	2.4	2.0
50	285.83	279.84	282.31	2.1	1.2
60	385.76	379.29	382.56	1.7	0.83
300	5603.75	5570.70	5593.02	0.59	0.19
600	17773.39	17712.18	17756.70	0.34	0.09
800	28699.42	28622.40	28681.00	0.27	0.06

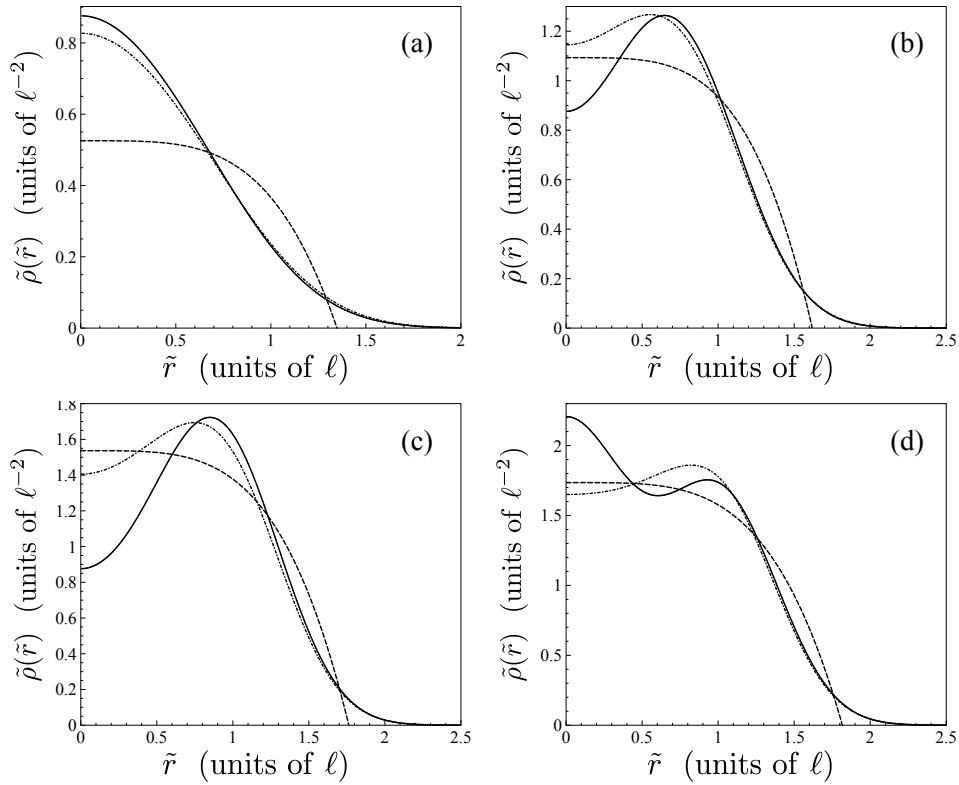
TABLE II: As in Table I, but for $\alpha = 4$.

FIG. 3: The spatial density, $\tilde{\rho}(\tilde{r})$ (scaled units) for the KS (solid curve), ADA (dot-dashed curve) and TF (dashed curve) evaluated at (a) $N = 2$, (b) $N = 6$, (c) $N = 10$ and (d) $N = 12$ particles with $\alpha = 4$. All quantities are scaled as discussed in the text.

reason, we have not presented the spatial densities and KE densities for these values of α , and simply state that curves similar to those found in Figs. 1-4 are found. It is comforting to note that the ADA continues to provide very good agreement in the tail region, even for large values of α (*i.e.*, steep confining potentials), indicating that the approximation is robust, and can provide accurate information about the properties of the system in the classically forbidden region (*e.g.*, this may be important in calculations of the binding energies, or atomic polarizabilities, where the results are sensitive to the spatial density distribution).

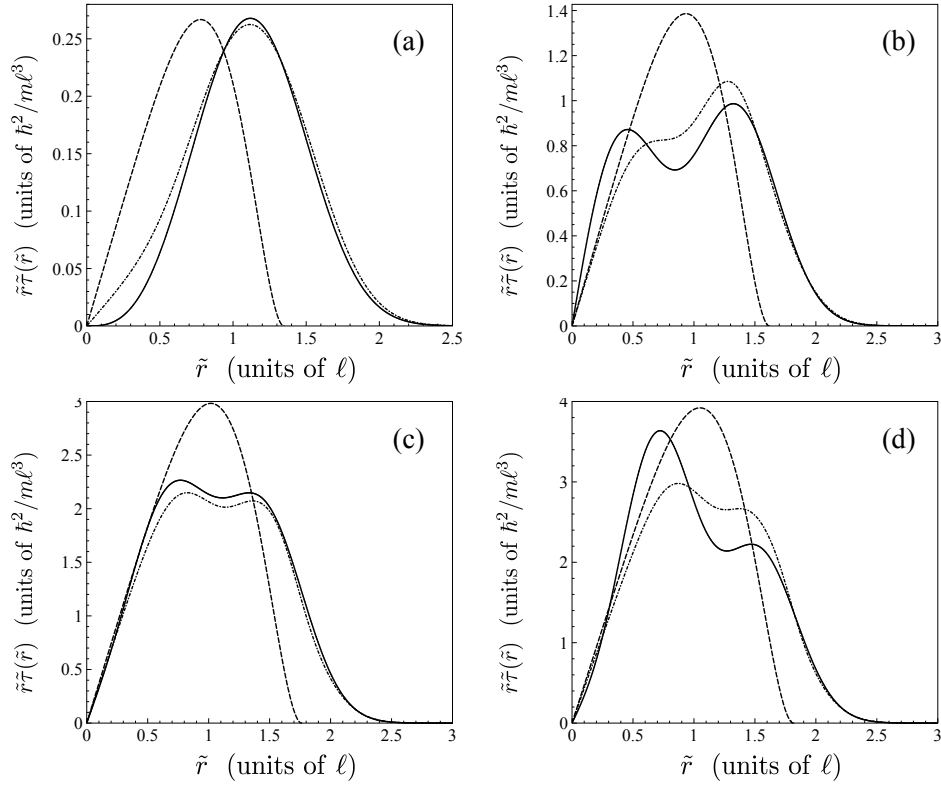


FIG. 4: The kinetic energy density, $\tilde{r}\tilde{\tau}(\tilde{r})$ (scaled units) for the KS (solid curve), ADA (dot-dashed curve) and TF (dashed curve) evaluated at (a) $N = 2$, (b) $N = 6$, (c) $N = 10$ and (d) $N = 12$ particles with $\alpha = 4$.

N	T_{KS}	$T_{\text{ADA}}[\rho_{\text{sc}}]$	$T_{\text{TF}}[\rho_{\text{TF}}]$	RPE^{ADA}	RPE^{TF}
2	1.96	2.15	1.50	9.7	23
6	11.40	11.37	10.29	0.26	9.7
10	27.64	26.30	25.15	4.9	9.0
12	36.60	35.72	34.60	2.4	5.5
16	60.67	58.18	57.24	4.1	5.7
20	87.73	85.27	84.58	2.8	3.6
50	427.98	417.74	420.40	2.4	1.8
60	585.55	574.35	578.41	1.9	1.2
300	9696.63	9624.13	9670.12	0.75	0.27
600	32572.81	32423.71	32526.3	0.46	0.14
700	42651.33	42476.65	42598.21	0.41	0.12

TABLE III: As in Table I, but for $\alpha = 6$.

B. Shifted Pöschl-Teller Potential

For our final potential, we will examine the so-called shifted Pöschl-Teller potential (PTP)[17], which can be written in the form

$$v_{\text{ext}}(r) = V_0[1 - \text{sech}^2(r/ar_0)] , \quad (25)$$

where $V_0 > 0$ is the depth, $r_0 > 0$ is the characteristic range of the potential, and $a > 0$ is a dimensionless constant. Equation (25) differs fundamentally from the power law potentials studied above, since it has only a finite number

N	T_{KS}	$T_{\text{ADA}}[\rho_{\text{sc}}]$	$T_{\text{TF}}[\rho_{\text{TF}}]$	RPE^{ADA}	RPE^{TF}
2	2.26	2.50	1.61	11	29
6	13.42	13.41	11.64	0.07	13
10	32.93	31.38	29.18	4.7	11
12	43.89	42.83	40.52	2.4	8
16	73.27	70.36	68.01	4.0	7
20	107.13	103.88	101.62	3.0	5.1
50	541.80	527.64	528.79	2.6	2.4
60	746.99	731.32	734.20	2.0	1.7
300	13351.06	13236.05	13303.20	0.86	0.36
700	61248.58	60940.60	61138.70	0.51	0.18
900	96247.39	95844.85	96111.64	0.42	0.14

TABLE IV: As in Table I, but for $\alpha = 8$.

of bound states owing to its saturation to the constant value, V_0 , as $r \rightarrow \infty$. The PTP also has uses in chemistry, where anharmonic potential energy surfaces are often needed for a realistic description of molecular dynamics, and in solid-state physics, where for example, the unshifted PTP, *viz.*, $v_{\text{ext}}(r) = -V_0 \text{sech}^2(r/ar_0)$, is often used to describe the “hole” produced by the diffusion of material species at double heterojunctions [18].

Scaling lengths by r_0 , and energies by \hbar^2/mr_0^2 provides the dimensionless form for Eq. (25),

$$\tilde{v}_{\text{ext}}(\tilde{r}) = \tilde{V}_0[1 - \text{sech}^2(\tilde{r}/a)] . \quad (26)$$

A series expansion of Eq. (26) about \tilde{r}/a contains even powers of \tilde{r}/a , implying that the PTP can be viewed as a linear combination of the even- α power-law potentials in Eq. (20). We choose the values $\tilde{V}_0 = 60$ and $a = 6$ so that (i) the decay of the spatial density is on the same order as the HO spatial density for similar particle numbers, and (ii) the potential can support enough bound states to contain the desired range of particle numbers listed in Table V.

N	T_{KS}	$T_{\text{ADA}}[\rho_{\text{sc}}]$	$T_{\text{TF}}[\rho_{\text{TF}}]$	E_{KS}	$E_{\text{ADA}}[\rho_{\text{sc}}]$	$E_{\text{TF}}[\rho_{\text{TF}}]$	RPE^{ADA}	RPE^{TF}
20	52.18	51.38	51.96	106.95	105.24	106.39	1.6	0.52
60	261.51	258.75	260.49	546.34	539.63	543.38	1.2	0.54
120	711.13	707.61	710.34	1514.57	1504.09	1510.61	0.69	0.26
240	1904.12	1899.00	1902.57	4169.03	4156.70	4166.98	0.30	0.05
520	5511.52	5509.30	5512.31	12745.38	12726.94	12742.00	0.14	0.03
670	7713.45	7712.60	7714.49	18297.86	18279.01	18295.41	0.10	0.01

TABLE V: Comparison of the exact KE, T_{KS} , and the exact KS total energy, E_{KS} , with the same quantities calculated *via* the ADA and TF calculations, under the PTP confinement, Eq. (25). The last two columns give the relative percentage error (RPE) between E_{KS} and $E_{\text{ADA}}[\rho_{\text{sc}}]$ and E_{KS} and $E_{\text{TF}}[\rho_{\text{TF}}]$, respectively. Energies are measured in units of \hbar^2/mr_0^2 .

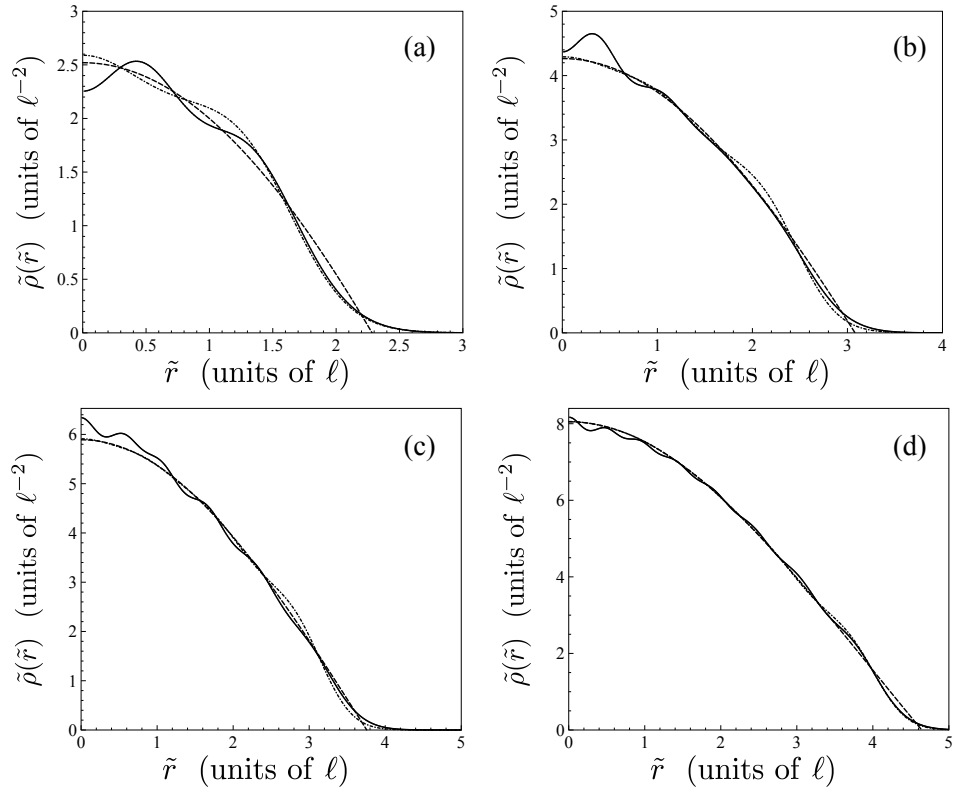


FIG. 5: The spatial density, $\tilde{\rho}(\tilde{r})$ (scaled units) for the KS (solid curve), ADA (dot-dashed curve) and TF (dashed curve) evaluated at (a) $N = 20$, (b) $N = 60$, (c) $N = 120$ and (d) $N = 240$ particles for the shifted PTP.

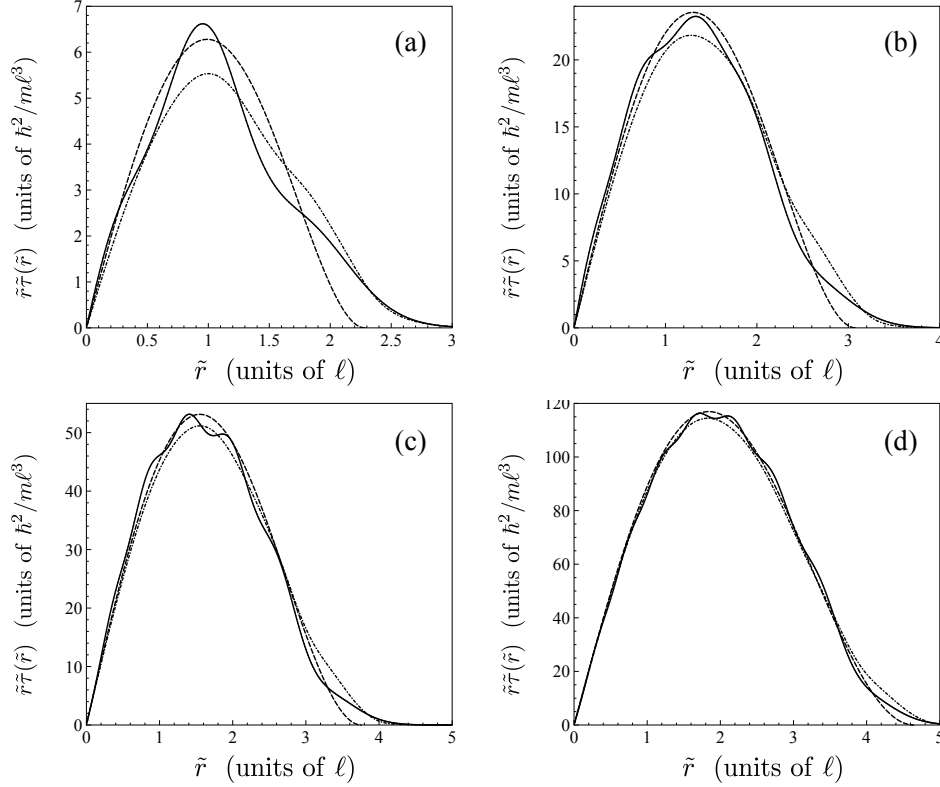


FIG. 6: The kinetic energy density, $\tilde{r}\tilde{\tau}(\tilde{r})$ (scaled units) for the KS (solid curve), ADA (dot-dashed curve) and TF (dashed curve) evaluated at (a) $N = 20$, (b) $N = 60$, (c) $N = 120$ and (d) $N = 240$ particles for the shifted PTP.

Table V provides a comparison between the exact KS energy, E_{KS} , and KE, T_{KS} , with the same quantities calculated *via* the ADA and TF approximation. Again, we observe the trend that the TF approximation yields very good agreement with the exact KS energy, and as we increase the number of particles, the TF approximation improves. By $N = 670$ particles, the RPE for the TF approximation is already better by an order of magnitude. Nevertheless, the TF approximation provides a comparatively inferior description of the spatial and KE densities as illustrated in Figs. 5 and 6; in contrast, the ADA continues to give an accurate description of the densities in the very low density regime. It is also apparent that the ADA spatial densities closely follow the TF approximation in the bulk, with the important difference of having a smooth decay into the classically forbidden region, in good agreement with the exact KS spatial density.

In Fig. 6, we observe that even though the spatial densities associated with the TF and ADA are quite similar (panels (b)-(d) in Fig. 5), the KE densities reveal some notable differences both within the bulk and the tail region. In particular, the ADA KE density does not capture the oscillatory behaviour of the KS KE density as well as in the power law potentials, which highlights the fact that the oscillations in the ADA are cannot be directly associated with the filling of the orbitals in the KS calculation.

IV. CLOSING REMARKS

We have provided a detailed examination of the efficacy of the recently proposed ADA for the KE functional of an inhomogeneous 2D Fermi gas. Our central finding is that while even the exceedingly simple TF KE functional can yield very good agreement with the exact KE of the system, it does a very poor job at providing the spatial and KE densities, especially at low particle numbers. Our findings also nicely illustrate that the 2D HO potential is a rather special case in 2D [14] (see also the discussion in Ref. [1]), and should not be the sole benchmark for testing the quality of any proposed KE functional for an inhomogeneous system. On the other hand, the ADA KE functional we have proposed for the 2D Fermi gas yields comparatively excellent agreement with exact KS calculations for the KE, as well as the local (*i.e.*, point-wise) densities, for a variety of trapping potentials. Our results demonstrate that the ADA provides an accurate, *parameter-free* KE functional which can be used with confidence in orbital-free DFT, even when the external potentials are tightly confining.

Finally, it would be of interest to implement the work of Kugler [19] to go beyond the linear-response condition leading to our ADA KE functional, and utilize the hierarchy of coupled equations presented in Ref. [19], which in principle fully determine the KE functional for an arbitrary inhomogeneous system. It is hoped that by including a truncated set of functional expressions, a closed system of equations can be solved, thereby developing an improved KE functional, and providing insight into constructing a truly universal expression for the KE functional, which can be implemented in an orbital-free density-functional theory.

Acknowledgments

This work was supported by grants from the Natural Sciences and Engineering Research Council of Canada (NSERC). W. Kirkby would like to thank the NSERC Undergraduate Summer Research Award (USRA) for additional financial support. B. P. van Zyl would like to thank E. Zaremba for useful discussions during the early stages of this work.

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